UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Chemistry of Molecular Materials

2425-2-F5401Q051

Aims

objectives

Molecular materials are rapidly gaining momentum, both in terms of scientific research and technological applications. Aim of the course is to provide a detailed knowledge of the structure properties relationships ruling the behaviour of such materials, with particular emphasis on electronic, optical and optoelectronic properties.

**Knowledge and understanding **

At the end of the course the student:

1. Understands the concept of conjugation in organic materials and correlates the extension of conjugation with optical, electrical and optoelectronical properties
2. Understands the concept of non-covalent bond and is capable of understanding its influence in the solution and solid-state aggregation behavior of organic materials
3. Can distinguish between electron donating and electron accepting residues in organic molecules. Can reason on their influence on electrical, optical and optoelectronical properties.
4. Can design organic conjugated materials for a specific purpose, given a series of conditions defining the required behaviour

Applying Knowledge and understanding:

The student:

1. Knows the basic working principles of organic electro/optic modulators, thin film transistors, electrochromic devices, solar cells, oleds, luminescent solar collectors, photodetectors. Based on such knowledge, the student is capable of proposing strategies to improve the performances of the same.
2. Knows the working principle of organic photoresists and can apply the concept in most documented industrial and research applications of the same

3. Is capable of independently gathering additional information on any one of the topics described during classes.
4. Knows and critically evaluates the literature of the field.
5. Understands the peer reviewing process and is capable of providing a report in the peer reviewing spirit

**Making judgments. **

Given the structure of a conjugated molecule or polymer, the student is capable of qualitatively estimating the corresponding optical, electrical and optoelectronical properties. On the other end, given a certain function that an organic molecule is required to perform, the student can propose known and original organic derivatives in principle capable of performing it. The student is also capable of estimating the influence of the environment on the properties of isolated ang aggregated molecules.

Communication skills.
The student is trained in the reading, understanding and summarizing of scientific literature. Particular emphasis is given to the capability of providing concise and complete information. The student possesses the specific terminology of the field, thus being in the position of discussing with counterparts possessing both a chemical and a physical/engineering background. He possesses a “problem solving” attitude.
Learning skills.
The Student is able to extend what has been learned in classes to case studies not covered during the course. He is in particular able to autonomously manage the wide literature dedicated to the conjugated materials. He knows the research tools of the dedicated literature, including patents.

Contents

Non-covalent interactions and molecular aggregates and solids: dipole-dipole, ion-dipole, hydrogen bonding, coordinative bonding and van der walls interactions. Examples of host guest interactions in solution: crown ethers, coronands, criptands, calixarenes and resorcinarenenes, rotaxanes and catenanes. Materials for nonlinearoptics: theoretical background. Molecular Materials for optoelectronics. Push-pull derivatives and BLA model. Bulk materials (poled polymers and sol-gel, Langmuir-Blodgett films, self assembled superlattices). Two-phonton absorbing materials and related applications (up converted lasing and imaging, optical limiting, 3D microfabrication) Synthesis and characterization of organic semiconductors. Transport properties in charge transfer complexes. Conducting polymers (polyacetylene, PPV, polyetherocycles). Electrochemical and oxidative polymerizations. Cross-coupling polymerizations.
Electrochromic materials and devices: background and design criteria for molecular and polymeric materials. Specific issues with devices assembly. Materials for displays and lighting: Working principle and device architecture of OLEDS. Molecular materials polymeric materials. Solid state down converting devices. Materials for organic solar cells. Organic rechargeable batteries. Elements of organic materials for bioimaging and photodynamic therapy.

Detailed program

The course is organized into classroom activities, guided reading activities, interactive classroom activities based on molecular design analysis and laboratory activities.

•Elements of conjugated materials design (building blocks)
•Elements of supramolecular chemistry (non covalent interactions)
•Conjugated molecules and materials having Nonlinear Optical Behavior
•Photoresists

•Organic polymeric semiconductors and conductors
•Electrochromic materials
•Organic Field Effect Transistors
•Scientific literature and databases
•Photodynamic therapy
•Organic solar cells (DSSC, perovskite, bulk heterojunction)
•Charge transfer complexes
•Organic light emitting devices

Students are inveted to take part to guided readings activites thus organized:

guided reading

• During classes you will have to repeat this exercise for few different papers
• Active discussions amongst fellow student in class will be organized.
•You will have to provide a referee report for a scientific paper that you assume is not in the final published form but rather at the submitted to the referees step

Design and critical analysis of molecular structures

• The work will be carried out in groups in the classroom and specific structures of molecules will be proposed and analysed. The structures will then be modified cooperatively to modify their intended properties.

Practical laboratory activity

• The work will be carried out in groups in the laboratory and some activities related to the preparation and characterization of devices will be proposed, experimenting with some techniques seen during the classroom lessons.

Prerequisites

Molecular based materials require an interdisciplinary approach. Elements of
•Materials science
•Organic chemistry
•Inorganic chemistry
•Physical chemistry
•Medicinal chemistry, environmental chemistry, physics…. (depending on the application) could be required

Teaching form

Teaching with different teaching methods:

11 two-hour and 1 one-hour lectures, in person, Delivered Didactics
2 two-hour seminar in in person about reading of scientific articles and discussion in the classroom, Interactive teaching
4 two-hour practical classes in person in delivery mode in the initial part which is aimed at involving students students interactively in the next part. Mixed teaching.
3 four-hour lab activities, in person, Interactive Teaching

Textbook and teaching resource

•Jonathan W. Steed, David R. Turner, Karl J. Wallace, Core Concepts in Supramolecular Chemistry and Nanochemistry, John Wiley&Son
•Nanoscale Science and Technology, R.Kelsal, I.Hamley, M.Geoghegan. John Wiley and Sons, Chichester, 2005
•Nanochemistry, G.A Ozin and A.C. Arsenault. Royal Society of Chemistry Publishing, Cambridge 2006.
•Kirk-Othmer encyclopedia of chemical technology (http://onlinelibrary.wiley.com/book/10.1002/0471238961)
•Annotated slides (on moodle)
•Registration of standard classes (on moodle)
•Video lessons (on moodle)

Semester

second semester.

Assessment method

•INTERVIEW ON THE TOPICS DEVELOPED IN LESSONS, ON THE EXAM TEXTS AND DISCUSSION ON THE LABORATORY ACTIVITIES.
•Evaluation of the guided readings assignments

during the exam the student will have to answer general questions on the topics discussed in both standard and video lesson. Questions will focus on the capability to reorganize the concepts discussed in classes. Students will be encouraged to reason on the possibile use of their notions in practical examples/aplications.

Office hours

generally in the afternoon between 14:30 and 17:30 but visits on appoitment are strongly suggested.

Sustainable Development Goals

QUALITY EDUCATION | AFFORDABLE AND CLEAN ENERGY | INDUSTRY, INNOVATION AND INFRASTRUCTURE